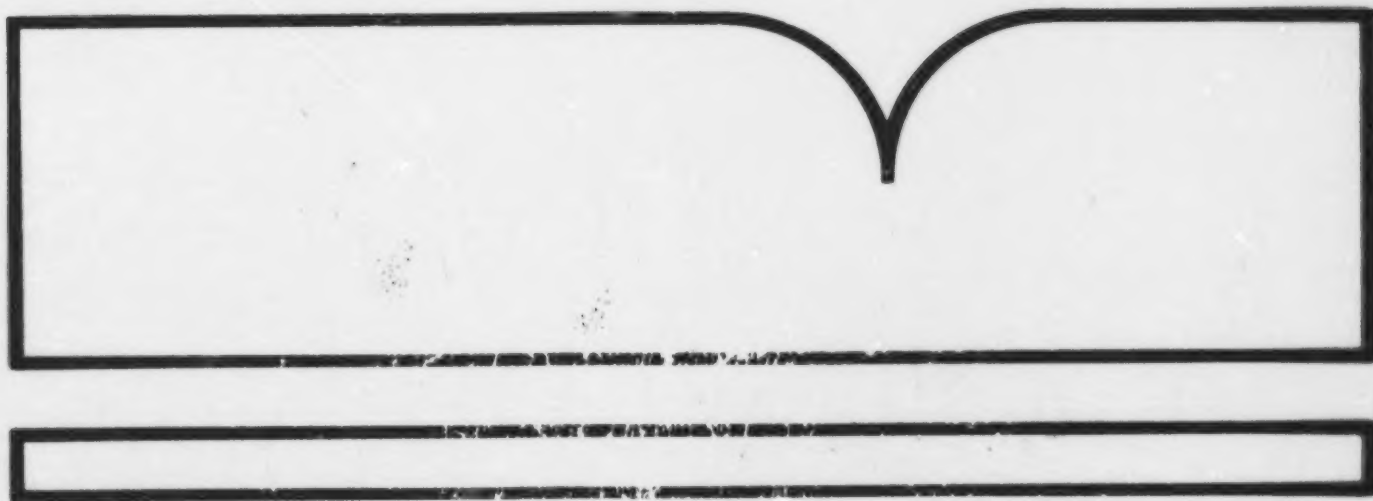


Chemical Information Systems
A Government Panel Review

Life Systems, Inc., Cleveland, OH

Prepared for
Environmental Protection Agency, Washington, DC

Aug 84



U.S. Department of Commerce
National Technical Information Service

NTIS

United States
Environmental Protection
Agency

Office of Information
Resources Management
Washington, DC 20460

August 1984
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Chemical Information Systems:

A Government Panel Review

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16. ABSTRACT The Chemical Information System (CIS) was initiated in 1971 by the Environmental Protection Agency and the National Institutes of Health. The CIS provides chemical information through computerized data bases to Government agencies and the public. EPA's Office of Information Resources management convened a Government Panel assembled a panel of thirteen experts representing Federal Agencies with interests in Chemical information to review CIS. This reports presents the recommendations resulting from the deliberations of the Panel.		
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CHEMICAL INFORMATION SYSTEMS:

A GOVERNMENT PANEL REVIEW

Prepared for the U.S. Environmental Protection Agency
Office of Information Resources Management

August 1984
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EXECUTIVE SUMMARY

Government Representatives were requested by the Environmental Protection Agency (EPA) to assemble as a panel of experts to review and discuss the Chemical Information System (CIS) and to make recommendations to EPA regarding the future direction of the system. All members of the panel represented agencies that have a direct interest in utilizing or supplying chemical information, or in the computer systems that facilitate access to, and the use of, information and data.

Concurrently, a Blue Ribbon Panel from the private sector was also convened by EPA to study and make recommendations on CIS. This panel's report was reviewed by the Government Panel before it made its final recommendations to EPA. The report of the Blue Ribbon Panel is entitled: The Chemical Information System: A Blue Ribbon Panel Review, and is available from the National Technical Information Service, order number PB 84-217777.

In addition to reviewing the Blue Ribbon Panel report, the Government Panel was specifically asked to examine the following:

- purpose of, and present and future need for, the system
- present ability of the system to meet this need
- funding levels and sources

Moreover, the Panel was asked to make recommendations on responsibility for management of the system.

After reviewing materials provided by EPA and meeting in three separate sessions, the Panel concluded that the Government should not continue to bear complete responsibility for the operation of CIS. It recommended to EPA that the system and/or its component parts be turned over to the private sector (meaning non-government) as soon as practical, with the Government retaining responsibility for the data it supplies to the system.

The Panel further recommended that another Government Agency be identified to represent Federal interests in issues related to chemical information, both data and specialized computer software. It recommended that the selected Agency be one that would represent the broadest possible scope of interest in computer-based chemical information systems.

CHEMICAL INFORMATION SYSTEM (CIS)

Lacking a general government policy for chemical information, Federal Government agencies still have a need for chemical data to support their activities in scientific review and analysis, policy-making, research and development, and regulation in such areas as the environment, public health and safety, food and nutrition, occupational health and safety, and consumer product safety. Government Agencies have recognized that it is in the public interest to disseminate chemical information collected or generated by the Government to all individuals and organizations that have a need for it, including other Government bodies, universities, research institutions, and private sector organizations. Such data sharing increases efficiency by reducing duplication in data gathering and maintenance, and also improves data quality by providing more opportunities for expert review of data.

Some of these data needs have been satisfied through the CIS managed by the EPA. The system has been sponsored by the EPA, The National Institutes of Health, The National Bureau of Standards, The Food and Drug Administration, and the Consumer Product Safety Commission.

This computer-based information system is composed of chemical data bases, some of which are Government-collected or -generated, and data analysis computer programs. The system contains numeric data in the areas of toxicology, environment, spectroscopy, chemical and physical properties, and allows for structure, substructure and full or partial name searching on over 300,000 unique chemical substances.

CIS is a very complex system. It is not the purpose of this report to provide a full description of the system. However, an overview of the system and its operation can be depicted in the three figures that follow. Figure 1 reflects the processing flow of the system and identifies major system elements. Figure 2 reflects the concept of data base integration through the Chemical Abstract Service (CAS) Registry Number and the Structure and Nonenclature Search System (SANSS) process. Figure 3 reflects the system functions and the organizations assigned responsibility for each function.

Additional information on the total system is available in various reports and papers produced in the last few years. A bibliography of the most pertinent publications is included in appendix F.

PRESENT CIS PROCESSING FLOW

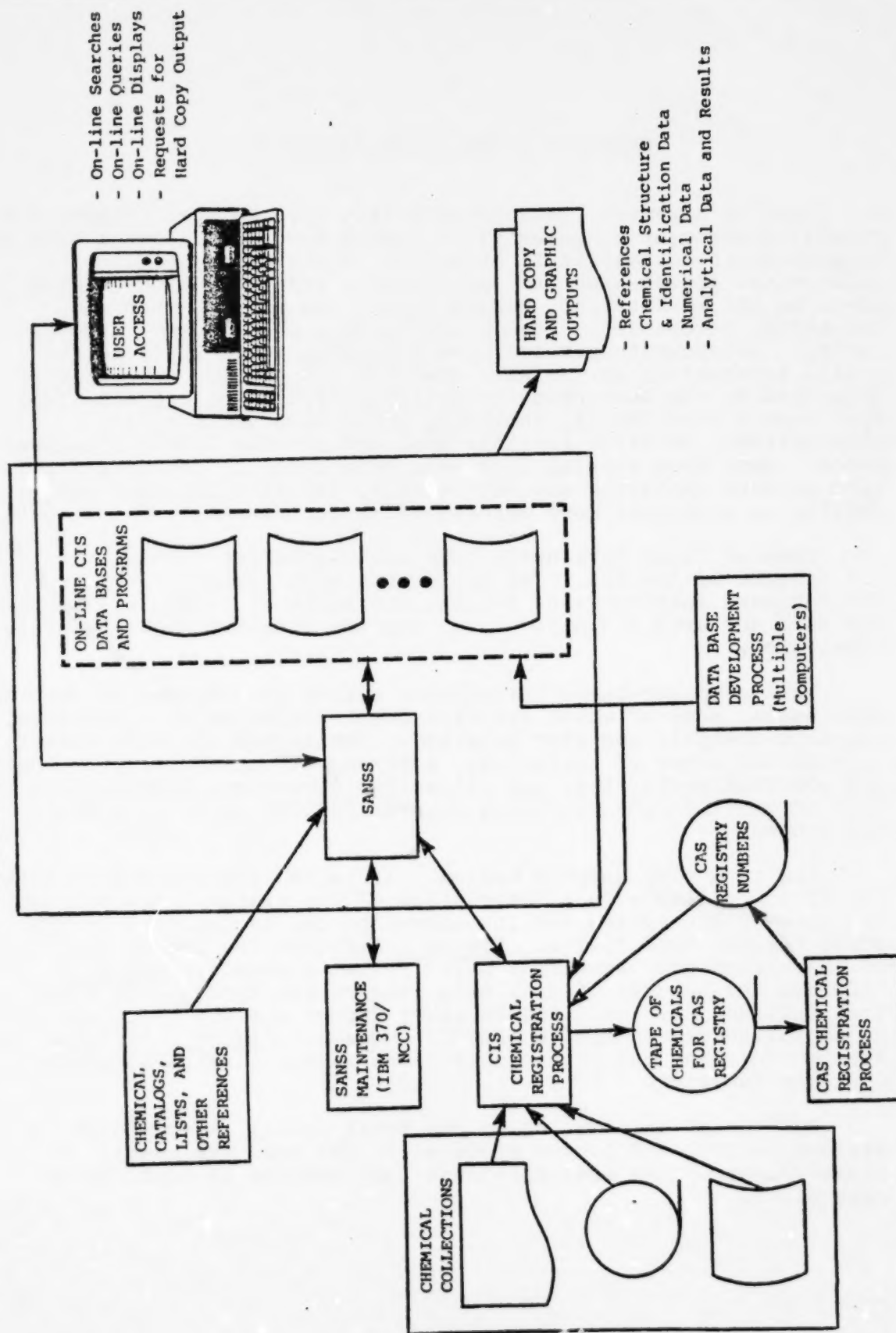


FIGURE 1

Data Base Integration Through SANNS

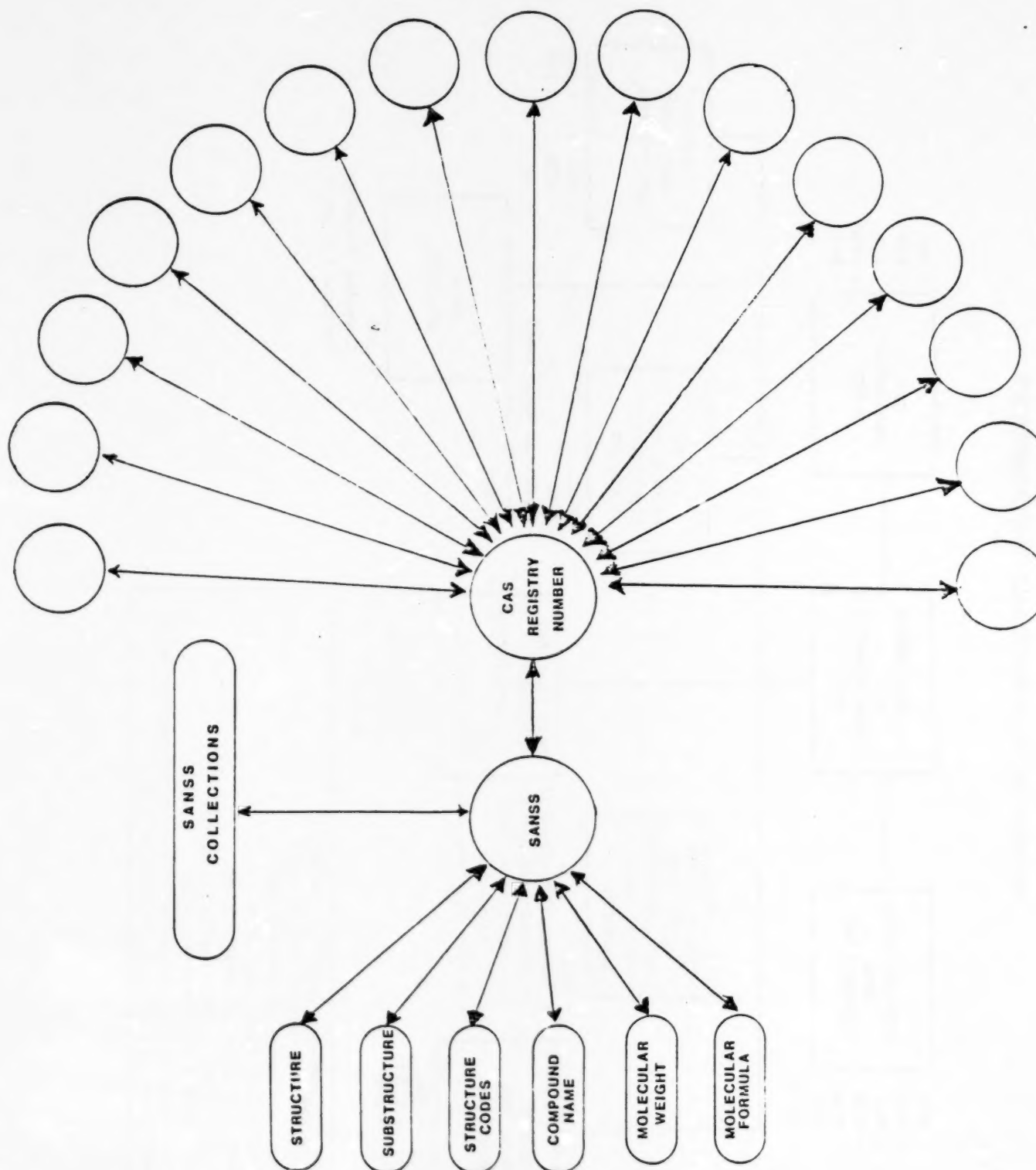


FIGURE 2

PRESENT CIS FUNCTIONS AND RESPONSIBILITIES

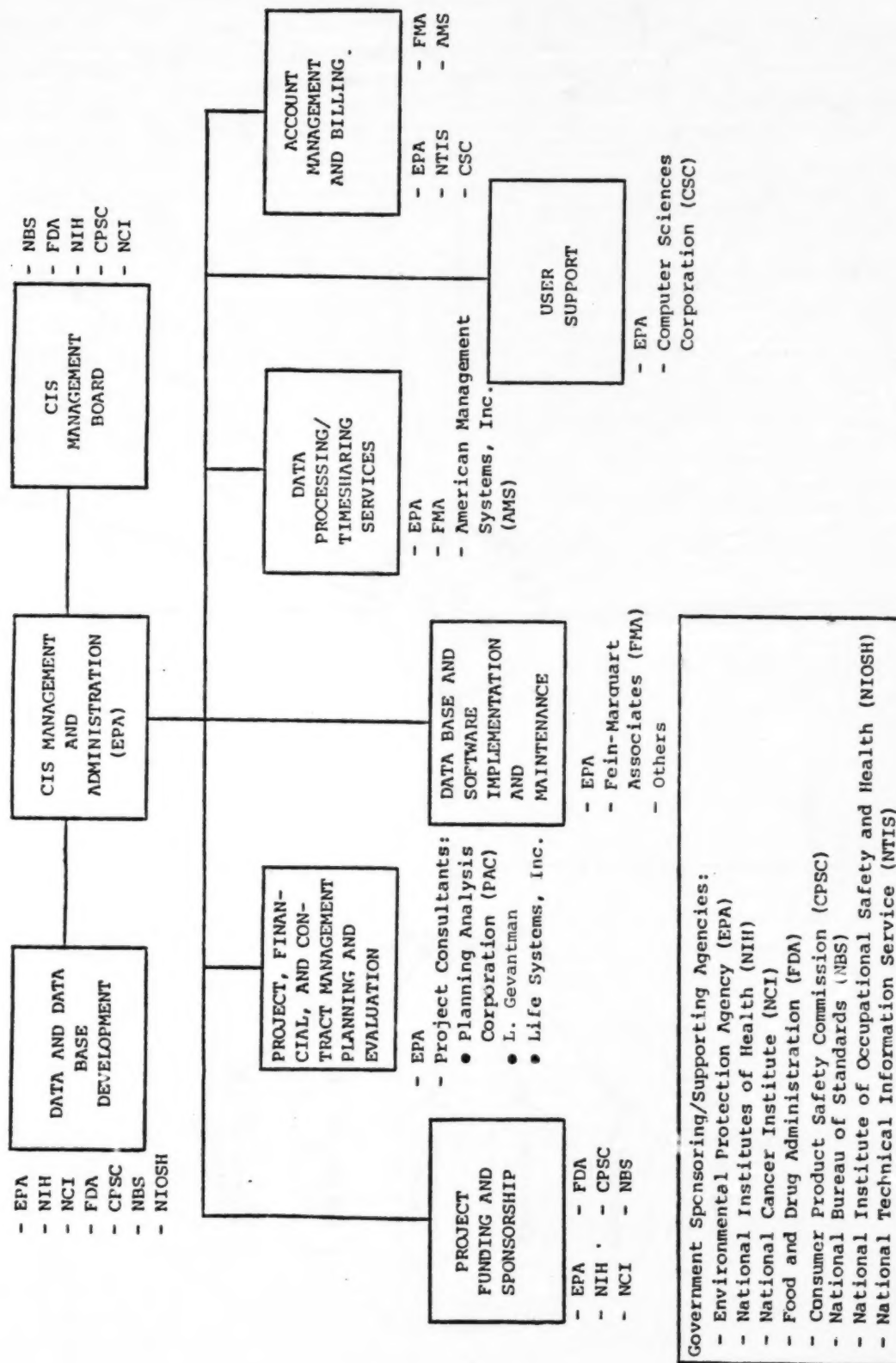


FIGURE 3

STATEMENT OF THE PROBLEM

The EPA, in its role as the Government manager of the CIS, has experienced increasing difficulties in monitoring the operation of the system. In an effort to overcome the difficulties and correct problems, EPA initiated a full review of the system late in 1983. The first task undertaken was to identify major overriding and crosscutting problems. Among those identified were:

- Lack of well-defined goals and objectives for the system - no clear conceptual framework
- Collaborative efforts and funding by several agencies leading to problems such as:
 - inability to assess true utility of system functions
 - lack of clear responsibility for ensuring accomplishment of tasks
 - difficulty exercising financial control
- Lack of well-defined and well-documented procedures for financial management, contracts management, data management and software development:
 - limited management resources available relative to number of contractor staff and dollar value of project - span of control problem
 - lack of adequate management information to support decision-making
- Large and increasing funding burden placed on EPA
- Lack of system flexibility, preventing needed changes to the system
- Lack of software documentation
- Growing user problems with the system
- Focus of EPA on toxic chemicals

Having identified these problems, it was evident to EPA that corrective action was necessary. While some actions were taken independently by EPA, others required the involvement of, or coordination with, other agencies. While not all inclusive or in any particular sequence, the following actions were taken by EPA:

- Requested full Office of the Inspector General audit of the system
- Reduced all contract activities to the absolute minimum pending resolution of the most critical problems
- Began a project to define and document procedures and controls for CIS financial management.
- Began audits of the data and data bases in late January 1984.
- Solicited offers of interest, from the private sector, to operate CIS.
- Began discussions with collaborating agencies' budget and information resources management (IRM) officials to tell them of CIS problems.
- Organized and conducted Government and private sector reviews of CIS.

This last action led to the establishment of the Government Panel to review the CIS and to make recommendations to EPA on further actions to be taken. See Appendix A for membership listing of the Government Panel, and Appendix B for the purpose of, and charge to, the Government Panel.

FINDINGS OF GOVERNMENT PANEL

The Government Panel held formal meetings on April 16, June 5, and July 13, 1984. The Honorable A. Alan Hill and Dr. Arthur F. Findeis served as Co-chairmen of the Panel. All meetings were well attended by either the principal or the alternate representative of the agencies, each of whom was knowledgeable regarding the CIS. Documentation on the CIS was provided by EPA and previous studies of the system were made available.

While it would not be practical to attempt to report the details of eight hours of intense discussions in a summary paper, the outcome of these discussions registered concerns which centered around the very need for the system and its operation. A number of other important questions were raised by the Panel:

- Are all the data bases included in CIS necessary?
The large amount of data included in the system contributes significantly to the operating cost.
- Should CIS include only data bases from those agencies who would agree to provide funding for a specified period of time?
- Should CIS contain only data bases that are updated on a regular schedule?
- Should CIS consist of only those data bases that could be linked to other data bases in the system?
- Can the quality of data be improved in the present CIS?
- Should CIS contain only Government-generated data bases? If not, how should private sector data bases be selected for inclusion?
- How important is it that data bases co-reside in a single system for the purposes of cross-file searching (i.e., through a SANSS-like capability)?
- Does the private sector have the capability to operate a CIS-like service?
- Is the current CIS software adequate for present and future needs?
- If the system is to be operated by the Government, which agency should serve as the lead agency?

- Does CIS meet the needs of participating agencies?
- Does the Government require the data in, and the processing capabilities of, CIS, to perform its mandated missions?

A poll of each Agency which provides data to CIS was conducted to determine whether its data bases (1) must be a part of CIS, (2) are preferable as a part of CIS, or (3) could be dropped from CIS. The results, included in Appendix E, reflect some need to reduce the present data base inventory.

The Panel concluded that, based on responses to the EPA's Commerce Business Daily notice, private sector organizations are capable of implementing a system comparable to CIS. Whether or not a private sector organization would be interested in implementing such a system depends on the answers to the following questions:

(1) What is the potential market and revenue for a CIS?

(2) Would the government be in competition with the private sector by continuing operation of CIS?

(3) What assurances would the private sector have for on-going availability of accurate data sources for the Government-sponsored data bases?

The Panel concluded that, once these questions were answered to the satisfaction of the private sector, one or more organizations would implement all or pieces of a system similar to CIS.

The Panel members felt strongly that any Government agency requiring little-used, non self-supporting data bases must operate them for their own use or must assume the costs to the private sector of loading and maintaining these data bases. Self-supporting, in this context, means that the revenue derived from user fees offsets operating costs.

As a result of its study and deliberations, the Panel found that:

- It is important to separate the task of gathering and analyzing data from the task of distributing the data. The Government has a responsibility to collect and validate its data, but operation of an on-line system, such as CIS, is not an inherent government responsibility.

- Most Panel members reported the existence of alternate sources for access to the data now provided to CIS by their agencies. However, in some instances, users determined their answers by combining various CIS data bases in their queries.
- CIS files and software have not been up-dated on a regular basis, creating a situation not easily corrected in the present system at a reasonable cost. CIS is a twelve year old system whose original unique features have been surpassed by rapidly moving technical developments in the handling of chemical data.
- The SANSS linkage across the various components in CIS is a unique and valuable characteristic of the system. Some members speculated that it might be five years before this functionality would exist in another system; others thought it would be available in much less time.
- Lacking policies on the quality and timeliness of information, many of the files in CIS contain inaccurate and badly out-of-date information.
- The expertise to effectively market the system is more easily available in the private sector.
- The computer hardware environment currently being used for CIS may not be supported by the manufacturer in the future.
- Some of the CIS files should not be maintained.
- The offers EPA had received from private sector organizations expressing an interest in operating CIS or a replacement for CIS confirmed the Panel's view that the capability to support a chemical information system presently exists in the private sector.
- A Systems Administrator and a Data Base Administrator, both with adequate supporting staff, would be required for EPA or any other Agency to properly manage CIS. Also, an advisory committee of technical experts would be needed. Finally, it would require identified funding sources to ensure economic viability to develop and implement both a short- and long-range plan for CIS.
- The findings and recommendations of the Blue Ribbon Panel Report were consistent with those of the Government Panel, with generally the same basic conclusions. Specific objections related to the inconsistencies in recommending that CIS be transferred to the private sector and at the same time recommending continued Government responsibility.
- The Panel concluded that little or no additional funding could be raised by the other current sponsors to replace the funding level now contributed by EPA.

GOVERNMENT PANEL RECOMMENDATIONS

The Government Panel Recommends To EPA:

1. That EPA turn CIS over to the private sector as soon as practical.
2. That the Blue Ribbon Panel Report is acceptable in principle with the following specific differences:
 - The Government Panel makes a clear distinction between data development and data distribution responsibilities.
 - The Government Panel disagrees with the conclusion that "the Government must continue to be responsible for assuring the existence of a publicly available system supplying chemical information".
3. That another agency administer the CIS activity until a final non-Government organization take-over is accomplished. It is recognized that adequate resources must be made available by EPA and other sponsoring agencies to ensure the viability and integrity of the system during the transition period.
4. That EPA make immediate contact with other sponsoring agencies to determine possible estimates of future financial support of a chemical information system.
5. That the above recommendations are all contingent upon a rational financial plan to support such a transfer in an orderly and responsible manner.

The Panel suggests that EPA involve the representatives of the sponsoring agencies, as well as others with major interest and responsibilities in chemical information, in the implementation of these recommendations.

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Appendix B

PURPOSE FOR AND CHARGE TO THE GOVERNMENT PANEL

After careful consideration of options available to review the Chemical Information System, EPA decided to assemble a Panel of Government Representatives to assist in the task. Panel members were selected from a wide variety of agencies having an interest in the System. The charge to Panel members was given to each member prior to the first meeting.

Charge to Government Panel Members

The Environmental Protection Agency considers data that impact health and environmental risk assessment of paramount importance. Over the past several years it has developed and supported a number of systems which provide chemical and other data in support of its missions. One of the systems is the Chemical Information System (CIS), a visible government activity in the area of chemical data handling. CIS is a collection of chemical data bases as well as data analysis computer programs. It contains numeric data in the areas of toxicology, environment, spectroscopy, chemical and physical properties, and allows for structure, substructure and full or partial name searching on over 300,000 unique chemical substances.

As the CIS has grown in size, cost, and complexity, the Agency wants to examine the need for such a system for the Agency as well as other governmental agencies. To this end the Agency is initiating a number of management actions to ensure the best use of its resources in continuing support of a chemical information system.

As government experts representing those agencies with an interest in Chemical Information you are being asked to review the present CIS system with emphasis on Government's need and responsibility for such a system.

Most importantly, after reviewing the materials provided, you are asked to:

- Review the purpose of, and need for, the system
- Review its present ability to meet this purpose
- Review the future need for the system
- Review its funding levels and sources
- Make recommendations concerning the responsibility for the management of the system.

You are also asked to provide input to the outside Blue Ribbon Panel of Experts as appropriate and to review its draft report. Recommendations from the panel should define the future course of CIS activities for the Government Agencies.

1.0 EXECUTIVE SUMMARY

The Chemical Information System (CIS) was initiated in 1971 by the Environmental Protection Agency (EPA) and the National Institutes of Health (NIH). The CIS provides chemical information through computerized data bases to government agencies and the public. At the request of the EPA Office of Information Resources Management (OIRM), ICAIR (Interdisciplinary Consulting and Information Research) of Life Systems, Inc. assembled a panel of nine experts to review CIS. The panel met at a symposium on June 11-13, 1984 to make recommendations for technical, financial and managerial improvements for CIS. The panel included experts in the following fields: chemistry, toxicology, numerical data, environmental and information science.

Overall, the panel concluded that CIS as a concept has considerable inherent value, however, improvements are necessary before CIS could serve the significant need for a high quality, integrated, scientific and technical chemical information system.

The panel reached unanimity of opinion on seven major topics: CIS purpose, capabilities, management problems, steps to become self-supporting, potential self-supporting files, government responsibilities and the management structure most appropriate for CIS. Briefly, the specific recommendations or consensus statements developed by the panel are as follows:

- After reviewing the demands for chemical information, the panel concluded that "...there is a need for a high quality, integrated scientific and technical system that is widely and easily accessible with manipulation and modeling capabilities."

The panel was informed by EPA that the original purpose of CIS (to provide mass spectral data) had never been formally revised, and that a more appropriate purpose was needed for the current system. Therefore, the panel proposed that "the purpose of CIS is to be an integrated system of chemical data (including both qualitative and quantitative data) which serves the needs of governmental agencies and the public for data on environmental and health effects and characteristic properties of chemical substances." The panel recommended that this purpose be adopted and serve as the focus for a new management strategy.

- The panel concluded that existing CIS capabilities and characteristics are inadequate to meet what they perceived are the demands for chemical information. Lack of consistency in mnemonics, terminology, educational and training materials highlight a list of deficiencies which reduce the effectiveness of CIS. However, the panel noted that the directory capability achieved by the Structure and Nomenclature Search System (SANSS) and the numeric data bases in CIS are exceptional.
- The panel judged that CIS data base selection, implementation and maintenance, systems standards, quality control, policy-making, management resources and public awareness are inadequate. Data base selection, implementation and public awareness of CIS require the most improvement.

- The panel concluded that CIS should not be required to become entirely self-supporting. Underutilized, but valuable data bases will need continued government support. However, many steps can and should be taken to make CIS more self-supporting than at present. These steps include: retrieval of more costs from users, improvement in operating efficiency, and increased utilization of the system.
- Although the panel agreed that all high use files presently on CIS could now be self-supporting if transferred to the private sector, such fragmentation of CIS as a system would have a detrimental impact to the ascribed purpose of providing an integrated system. As long as CIS can be improved to meet the specifications developed by the panel, high use files should not be separated. This does not preclude concurrent availability of high use files in the private sector which might be a source of additional revenue to CIS.
- In the panel's view, the government must continue to be responsible for assuring the existence of a publicly available system supplying chemical information. This responsibility should be implemented through a new management strategy capable of correcting the major problems and enhancing the ability of CIS to serve its purpose.
- The panel concluded with a recommendation that a more appropriate management concept for CIS be adopted. The panel's recommendation for this concept consists of a management role for the government and a separate implementation role. For the management role within the government the panel recommended EPA, the National Library of Medicine (NLM) or the Council on Environmental Quality (CEQ), in that order of preference. The panel recommended NLM, a professional society, or a private data base vendor as viable candidates for the implementation role. As second choices, but also viable candidates, the panel recommended a privately operated government laboratory or a private research institute.

APPENDIX 1

TR-576-42B

LIST OF PARTICIPANTS

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(a) Designated alternate spokesperson for the panel.

(b) Designated spokesperson for the panel.

AGENCY DATA BASE REVIEW

The Government Panel requested EPA to obtain specific information on each of the data bases included in CIS. Sponsoring agencies were asked to answer ten questions. Results are reflected below:

CIS AGENCY DATA BASE REVIEW

DATA BASE	SANSS Desirable	Reside w/other files on CIS	On Line	24 Hour Day	Up-Dated by Sponsors	Up-Dated by Other	of value if not Up-Dated	Available elsewhere	Would sponsor make available if no CIS	Drop from CIS
1. Arthur		N	Y	N	Y	N	Y	Y	N	N
2. FRSS	Y	Y	Y	N	N	Y	Y	N	N	N
3. CTCP (FDA)	Y	Y	Y	Y	Y	Y	Y	Y	N	N
4. MSSS (FDA)	Y	Y	Y	Y	N	Y	Y	N	N	N
5. CTCP (CPSC)					N	Y	Y	Y	N	Y
6. MSSS (NBS)	Y	N	Y	N	Y	Y	Y	Y	Y	N
7. Thermo	Y	N	N	N	Y	Y	Y	Y	Y	N
8. Xtal	Y	N	Y	N	Y	Y	Y	Y	Y	N
9. CRYST	Y	N	Y	N	N	Y	N	N	Y	N
10. CNMR	Y	N	N	N	N	Y	Y	N	N	Temp
11. NMRLIT	N	N	N	N	Y	Y	N	N		Temp
12. MLAB	N	N								Y
13. CLAB	N	N								Y
14. CCRIS	N	N								Y
15. OHMTADS	Y	Y	Y	Y	Y	N	Y	N	Y	N
16. EPACASR	Y	N	Y	N	Y	Y	Y			N
17. IPIS	N	N	Y	N	Y		N	N		N
18. SPHERE	Y	Y	Y	N	Y	Y	Y	N	Y	N

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1982 120P.; PAPERS ORIGINALLY PRESENTED TO THE DAVIS REFERENCE
SERVICES GROUP.

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AUTHOR (S): MILNE, G.W.A.
LOCATION: INFORM. TECHNOL. BRANCH, NATL. CANCER INST., BETHESDA, MD,
20205, USA
JOURNAL: J. ASSOC. OFF. ANAL. CHEM. DATE: 1982 VOLUME: 65 NUMBER: 5
PAGE: 1249-58

THE DEVELOPMENT AND EVOLUTION OF A CHEMICAL INFORMATION SYSTEM
AUTHOR(S): HELLER, S.R.
LOCATION: EPA, WASHINGTON, D.C. USA
JOURNAL: STUD. PHYS. THEOR. CHEM. DATE: 1981 VOLUME: 16 NUMBER: DATA
PROCESS. CHEM. PAGES: 164-85

ENVIRONMENTAL USES OF THE NIH-EPA CHEMICAL INFORMATION SYSTEM
AUTHORS (S): MILNE, G.W.A.: FISK, C.L.: HELLER, STEPHEN R.: POTENZONE
RUDOLPH, JR.
LOCATION: NATL. CANCER INST., BETHESDA, MD, 20205, USA
JOURNAL: SCIENCE (WASHINGTON, D.C., 1883-) DATE: 1982 VOLUME: 215
NUMBER: 4531 PAGES: 371-5

CREATION AND CAPABILITIES OF COMPUTERIZED DATA BANKS CONTAINING
INFORMATION ON CHEMICAL STRUCTURES AND PROTEINS
AUTHOR(S): HELLER, S.R.: MILNE, G.W.A.
LOCATION: EPA, WASHINGTON, DC, 20460, USA
JOURNAL: CODATA BULL. DATE: 1981 VOLUME: 40 PAGE: 41-4

THE NIH-EPA CHEMICAL INFORMATION SYSTEM (CIS)
AUTHOR(S): HELLER, S.R.: MILNE, G.W.A.
LOCATION: EPA, WASHINGTON, DC, 20460, USA
JOURNAL: PROC. INT. CODATA CONF. DATE: 1981 VOLUME: 7TH NUMBER: DATA
SCI. TECHNOL. PAGES: 343-6

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AUTHOR(S): DIJS, C.M.
LOCATION: NETH.
JOURNAL: CHEM. MAG. (THE HAGUE) DATE 1981 NUMBER: JUNE PAGES: 349-50
AUTHORS(S): HELLER, STEPHEN R.; MILNE, GEORGE W.A.

THE NIH/EPA CHEMICAL INFORMATION SYSTEM
AUTHOR(S): MILNE, G.W.A.: HELLER, S.R.: HELLER, R.S.; MARTINSEN, D.
P.
LOCATION: ADV. MASS SPECTROM. DATE 1980 VOLUME: 8B, PAGES: 1578-81

THE NIH/EPA CHEMICAL INFORMATION SYSTEM

AUTHOR (S): MILNE,G.W.A.:HELLER,S.R.

LOCATION: NIH, BETHESDA,MD,20502,USA

JOURNAL:J.CHEM.INF.COMPUT.SCI.DATE: 1980 VOLUME:20 NUMBER:4

PAGES: 204-11

CIS SYSTEMS FOR RETRIEVAL OF DATA ON CHEMICAL SUBSTANCES SAFETY

AUTHOR(S): ANON

LOCATION: JAPAN

JOURNAL: SUMITOMO KAGAKU TOKUSHUGO DATE: 1980 VOLUME:20 NUMBER:4

THE NHI/EPA CHEMICAL INFORMATION SYSTEM IN SUPPORT OF STRUCTURE ELUCIDATION

AUTHOR(S): HELLER, STEPHEN R.;MILNE, GEORGE W.A.

LOCATION: ENVIRO.PROT. AGENCY,WASHINGTON,DC,20460,USA

JOURNAL: ANAL.CHIM. ACTA DATE: 1980 VOLUME: 122 NUMBER:2 PAGES:117-38

THE NIH EPA/CHEMICAL INFORMATION SYSTEM

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THE NIH/EPA CHEMICAL INFORMATION SYSTEM

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